

Taurocyamine

543-18-0 | DTXSID10202654

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 189 °C

Global applicability domain: Inside

Local applicability domain index: 2.83e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Cartap hydrochloride</div> <div>Measured: 180</div> <div>Predicted: 184</div>	<div>Image not found</div> <div>Nalpha-Acetyl-L-glutamine</div> <div>Measured: 197</div> <div>Predicted: 192</div>	<div>Image not found</div> <div>Sulfathiourea</div> <div>Measured: 182</div> <div>Predicted: 189</div>
<div>Image not found</div> <div>Floxuridine</div> <div>Measured: 151</div> <div>Predicted: 170</div>		